1,4-Dioxane-2,3-diol, chlorodifluoroacetate, heptafluorobutyrate

Inchi: InChI=1S/C10H6ClF9O6/c11-8(14,15)6(22)26-4-3(23-1-2-24-4)25-5(21)7(12,13)9(16,17)

InchiKey: DCXLEOJHCZHVPA-UHFFFAOYSA-N

Formula: C10H6ClF9O6

SMILES: O=C(OC1OCCOC1OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)Cl

Mol. weight [g/mol]: 428.59

Physical Properties

Property code	Value	Unit	Source
gf	-2343.88	kJ/mol	Joback Method
hf	-2785.08	kJ/mol	Joback Method
hfus	38.35	kJ/mol	Joback Method
hvap	57.15	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.436		Crippen Method
mcvol	195.690	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
tb	667.50	K	Joback Method
tc	847.81	K	Joback Method
tf	447.97	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.66	J/mol×K	667.50	Joback Method
cpg	591.59	J/mol×K	697.55	Joback Method
cpg	601.61	J/mol×K	727.60	Joback Method
cpg	610.77	J/mol×K	757.65	Joback Method
cpg	619.10	J/mol×K	787.70	Joback Method
cpg	626.67	J/mol×K	817.76	Joback Method
cpg	633.52	J/mol×K	847.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375756&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume